

$\text{Ca}_4\text{Ag}(\text{Ag}_{0.2}\text{Si}_{0.8})_3\text{Si}_{3.2}$ $hP24$ $(187) P-6m2 - nk^2j^2hfeba$ **Ca₈Ag_{3.2}Si_{11.24}** [1]

Structural features: 3D-framework of fused Ca₆ trigonal prisms centered by Si, (Si,Ag) and Ag (partial vacancies ignored). Substitution derivative of AlB₂.

Merlo F. et al. (1996) [1]

 $\text{Ag}_{1.60}\text{Ca}_4\text{Si}_{5.62}$ $a = 0.8304, c = 0.8643 \text{ nm}, c/a = 1.041, V = 0.5161 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ca1	6 <i>n</i>	. <i>m</i> .	0.83347	0.16653	0.2504		pseudo Frank-Kasper Si ₁₀ Ag ₂ Ca ₈
M2	3 <i>k</i>	<i>mm</i> 2	0.16667	0.83333	$\frac{1}{2}$		tricapped trigonal prism Si ₃ Ca ₆
M3	3 <i>k</i>	<i>mm</i> 2	0.50067	0.49933	$\frac{1}{2}$		tricapped trigonal prism Si ₃ Ca ₆
Si4	3 <i>j</i>	<i>mm</i> 2	0.17457	0.82543	0		tricapped trigonal prism Si ₂ AgCa ₆
Si5	3 <i>j</i>	<i>mm</i> 2	0.49367	0.50633	0	0.48	tricapped trigonal prism Si ₂ AgCa ₆
Ca6	2 <i>h</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2488		pseudo Frank-Kasper Si ₁₂ Ca ₈
Si7	1 <i>f</i>	-6 <i>m</i> 2	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		tricapped trigonal prism Si ₃ Ca ₆
Ag8	1 <i>e</i>	-6 <i>m</i> 2	$\frac{2}{3}$	$\frac{1}{3}$	0		tricapped trigonal prism Si ₃ Ca ₆
Si9	1 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{2}$		tricapped trigonal prism Si ₃ Ca ₆
Ag10	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		tricapped trigonal prism Si ₃ Ca ₆

 $M2 = 0.77\text{Si} + 0.23\text{Ag}; M3 = 0.83\text{Si} + 0.17\text{Ag}$ Transformation from published data: origin shift $\frac{1}{3} \frac{2}{3} 0$

Experimental: single crystal, diffractometer, X-rays, wR = 0.096

References: [1] Merlo F., Pani M., Fornasini M.L. (1996), J. Alloys Compd. 232, 289-295.